UNIVERSITI PUTRA MALAYSIA

BLOCK BACKWARD DIFFERENTIATION ALPHA-FORMULAS FOR SOLVING STIFF ORDINARY DIFFERENTIAL EQUATIONS

ISKANDAR SHAH BIN MOHD ZAWAWI

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By

ISKANDAR SHAH BIN MOHD ZAWAWI

Thesis Submitted to the School of Graduate Studies, Universiti Putra Malaysia, in Fulfilment of the Requirements for the Degree of Doctor of Philosophy

March 2017

DEDICATIONS

To my beloved family members,

Mohd Zawawi Abdullah

Rozita Arifin

Anis Syazween

Noreen Natasha

Muzzaffar Shah

Alauddin Shah

and my supervisor,

Assoc. Prof. Dr. Zarina Bibi Ibrahim

for their support and patience.

Either mathematics is too big for the human mind or the human mind is more than a machine

Abstract of thesis presented to the Senate of Universiti Putra Malaysia in fulfilment of the requirement for the degree of Doctor of Philosophy

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March 2017

Chair: Zarina Bibi Binti Ibrahim, PhD
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A new family of block methods, namely block backward differentiation alpha-formulas (BBDF-α) are developed for solving first and second order stiff ordinary differential equations (ODEs) directly. By selecting the appropriate values of parameter α that can be controlled by user, the derived methods give better approximation compared to the existing methods. Initially, the derivation of BBDF-α using constant and variable step size approach for solving first order stiff ODEs is presented. The consistency and zero stability that lead to the convergence properties are discussed theoretically. Meanwhile, the stability regions are displayed to show that the derived methods are A-stable for certain values of α. Numerical results reveal the superiority of the derived formulas in terms of total number of steps, accuracy and computation time.

Subsequently, the BBDF-α is constructed for solving second order stiff ODEs directly. This method is specially designed to cater the second order ODEs without reducing it into the first order. The convergence aspects are investigated and the stability region is illustrated to verify the suitability of the method in solving stiff problems. Numerical results demonstrate the advantage of the method in terms of execution time due to its capability as direct solver. Furthermore, the BBDF-α is formulated using variable step size scheme for solving second order stiff ODEs directly. In order to describe the whole process of implementation, the numerical algorithm is exhibited. The results indicate that the developed method has advantage in terms of accuracy and total number of step. Finally, the application of derived methods in damped oscillation problems is presented. To test the performance of the methods, several experiments on over-damped, critically-damped and under-damped oscillation in mass-spring systems are conducted. In conclusion, the derived methods can be used as viable alternative solver for stiff ODEs and real-life problem.

Abstrak tesis yang dikemukakan kepada Senat Universiti Putra sebagai memenuhi keperluan untuk ijazah Doktor Falsafah

FORMULA-ALFA BLOK PEMBEZAAN KE BELAKANG BAGI MENYELESAIKAN PERSAMAAN PEMBEZAAN BIASA KAKU

Oleh

ISKANDAR SHAH BIN MOHD ZAWAWI

Mac 2017

Pengerusi: Zarina Bibi Binti Ibrahim, PhD
Fakulti: Sains

Keluarga baru kaedah blok iaitu formula-alfa blok pembezaan ke belakang (FBPB-α) dibangunkan bagi menyelesaikan persamaan pembezaan biasa (PPB) kaku peringkat pertama dan kedua. Dengan memilih nilai parameter α yang sesuai yang boleh dikawal oleh pengguna, kaedah yang diterbitkan memberi penghampiran yang lebih baik daripada kaedah sedia ada. Pada mulanya, penerbitan FBPB-α menggunakan pendekatan saiz langkah malar dan berubah bagi menyelesaikan PPB kaku peringkat pertama dibentangkan. Konsistensi dan kestabilan sifar yang membawa kepada sifat-sifat penumpuan dibincangkan secara teori. Sementara itu, rantau-rantau kestabilan dipaparkan untuk menunjukkan kaedah yang diterbitkan adalah A-stabil bagi nilai-nilai α tertentu. Keputusan berangka mendedahkan keunggulan kaedah-kaedah yang diterbitkan dalam terma jumlah bilangan langkah, kejituan dan pengiraan masa.

Seterusnya, FBPB-α dibina bagi menyelesaikan PPB kaku peringkat kedua secara langsung. Kaedah ini direka khas untuk memenuhi PPB peringkat kedua tanpa menurunkannya kepada peringkat pertama. Aspek penumpuan diselidik dan rantau-rantau kestabilan diilustrasikan untuk mengesahkan kesesuaian kaedah dalam menyelesaikan masalah-masalah kaku. Keputusan berangka menunjukkan kelebihan kaedah dalam terma pengiraan masa disebabkan keupayaannya sebagai penyelesai langsung. Selain itu, FBPB-α diformulasi menggunakan skim saiz langkah berubah bagi menyelesaikan PPB kaku peringkat kedua secara langsung. Untuk menerangkan keseluruhan proses perlaksanaan, algoritma berangka dipamerkan. Keputusan menunjukkan kaedah yang dibangunkan mempunyai kelebihan dalam terma kejituan dan jumlah bilangan langkah. Akhir sekali, aplikasi kaedah-kaedah dibangunkan dalam masalah-masalah ayunan teredam dibentangkan. Untuk menguji prestasi kaedah, beberapa eksperimen terhadap teredam lebih, teredam kritikal dan teredam bawah ayunan dalam sistem jisim-spring dijalankan. Kesimpulannya, kaedah yang diterbitkan boleh digunakan sebagai penyelesai alternatif berdaya maju bagi PPB kaku dan masalah kehidupan sebenar.

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I certify that a Thesis Examination Committee has met on 22 March 2017 to conduct the final examination of Iskandar Shah bin Mohd Zawawi on his thesis entitled "Block Backward Differentiation Alpha- Formulas for Solving Stiff Ordinary Differential Equations" in accordance with the Universities and University Colleges Act 1971 and the Constitution of the Universiti Putra Malaysia [P.U.(A) 106] 15 March 1998. The Committee recommends that the student be awarded the Doctor of Philosophy.

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Declaration by graduate student

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LIST OF ABBREVIATIONS

ODEs	:	Ordinary differential equations
IVPs	:	Initial value problems
LMM	:	Linear multistep method
BDF	:	Backward differentiation formula
NDFs	:	Numerical differentiation formulas
BBDF	:	Block backward differentiation formula
MEBDFs	:	Modified extended backward differentiation formulas
BDF-α	:	Backward differentiation α-formula
HHT-α	:	Hilber-Hughes-Taylor method
BBDF-α	:	Block backward differentiation α-formula
BBDF(3)-α	:	Block backward differentiation α-formula of order 3 for solving first order stiff ODEs
BBDF(4)-α	:	Block backward differentiation α-formula of order 4 for solving first order stiff ODEs
VSBBDF(3)-α	:	Variable step block backward differentiation α-formula of order 3 for solving first order stiff ODEs
VSBBDF(4)-α	:	Variable step block backward differentiation α-formula of order 4 for solving first order stiff ODEs
BBDF2-α	:	Block backward differentiation α-formula for solving second order stiff ODEs directly
VSBBDF2-α	:	Variable step block backward differentiation α-formula for solving second order stiff ODEs directly
BBDF(5)		2-point block backward differentiation formula of order 5
BEBDF	:	2-point block extended backward differentiation formula
3BEBDF	:	3-point block extended backward differentiation formula
2OBBDF	:	2 off-step points block backward differentiation formula
2PBOSM	:	2-point block one-step method
VSBBDF(3)	:	Variable step block backward differentiation formulas of order 3
VSBBDF(4)	:	Variable step block backward differentiation formulas of order 4
VSVOBBDF	:	Variable step variable order block backward differentiation formula for solving first order stiff ODEs
BBDF2	:	Block backward differentiation formulas for solving second order stiff ODEs directly
VSVOD	:	Variable step variable order direct integration method
BVSD	:	Block variable step direct integration method
VSVOBBDF2	:	Variable step variable order block backward differentiation formula for solving second order stiff ODEs directly
ode15s	:	Variable order method of numerical differentiation formulas of order 1-5
ode23s	:	Fixed order method of new modified Rosenbrock (2,3) pair
LTE	:	Local truncation error
h	:	Step size
SS	:	Total of successful steps
FS	:	Total of failure steps
MAXE	:	Maximum error
AVER	:	Average error
TIME	:	Execution time

CHAPTER 1

INTRODUCTION

1.1 Introduction

Differential equations have long been an essential part in most branches of physical sciences and engineering all over the world. Scientists and engineers often study the changes of variables in a system of equations to gain a deeper understanding of the underlying phenomena. One of the most well known differential equations is ordinary differential equations (ODEs) which can be categorized into stiff and non-stiff. In real life situations, the undamped and damped oscillation problems like mass-spring system are often modeled as second order ODEs. However, it is unfortunate that the majority of ODEs encountered in practice is difficult or impossible to be solved analytically. For this reason, a suitable numerical method must be derived where the approximated solutions are produced in the form of a graph or a table of numbers.

Nowadays, various accurate and efficient numerical methods are available to give a reasonable degree of confidence in the solution of ODEs. Numerical method can be classified as one step method and multistep method. For instance, the Runge-Kutta method is one step method, whereas the backward differentiation formula (BDF) is the method in the family of linear multistep method (LMM). The one step method is used to approximate the solution using one previous point while the multistep method computes the solution using several previous points. Since the BDF method is important in dealing with stiffness, here the attention will be directed towards the phenomenon of LMM which is confined to the new class of block backward differentiation formulas (BBDF) for solving stiff ODEs and some applied problems.

1.2 Problem statement

The dynamic behavior of any systems in real-life can be described in the form of ODEs. In this thesis, the numerical solution of ODEs is presented. The attention will be focused on solving single, system, first order linear and non-linear ODEs. Then the numerical method is extended to solve second order ODEs directly. It has to be pointed out that for all initial value problems (IVPs), there may exist analytical solutions. The general form of first order ODEs is defined as

$$y' = f\left(x, y\right), \quad y\left(a\right) = \eta \tag{1.1}$$

where the interval is $x \in \left[a, b\right]$. The order of ODEs is the order of the highest differential coefficient appears in the equation. Hence, the general form of second order ODEs is given by

$$y_i'' = f_i\left(x, y_i, y_i'\right), \quad i = 1, 2, \ldots, s, \tag{1.2}$$

where $y_i\left(a\right) = \eta_i$ and $y_i'\left(a\right) = \eta_i'$ are initial conditions with the interval $\left[a, b\right]$.

Equation (1.2) can be reduced to the system of first order ODEs as follows:

$$y'_{i,1} = y_{i,2}, \quad y'_{i,2} = f_i\left(x, y_{i,1}, y_{i,2}\right), \tag{1.3}$$

which is equivalent to

$$\tilde{Y}' = F\left(x, \tilde{Y}\right), \quad \tilde{Y}(a) = \tilde{\eta}$$

where

$$\tilde{Y}' = \left(y'_{1,1}, y'_{1,2}, \cdots, y'_{s,1}, y'_{s,2}\right)^T, \ \tilde{Y} = \left(y_{1,1}, f_1\left(x, y_{1,1}, y_{1,2}\right), \cdots, y'_{s,1}, f_s\left(x, y_{s,1}, y_{s,2}\right)\right)^T,$$

$$\tilde{Y}(a) = \left(\eta_{1,1}, \eta_{1,2}, \cdots, \eta_{s,1}, \eta_{s,2}\right)^T.$$

Throughout the thesis, the following theorem which states the conditions on $f\left(x, \tilde{Y}\right)$ guarantee the existence of a unique solution of (1.1).

Theorem 1.1
Let $f\left(x, \tilde{Y}\right)$ be defined and continuous for all points $\left(x, \tilde{Y}\right)$ in the region D defined by $a \le x \le b$, $\|\tilde{Y}\| < \infty$, where a and b are finite, and let there exists a constant L known as Lipschitz constant such that for every $x, \tilde{Y}$ and $\tilde{Y}^*$ such that $\left(x, \tilde{Y}\right)$ and $\left(x, \tilde{Y}^*\right)$ are both in D,

$$\left\| f\left(x, \tilde{Y}\right) - f\left(x, \tilde{Y}^*\right) \right\| \le L \left\| \tilde{Y} - \tilde{Y}^* \right\|. \tag{1.4}$$

Then it $\tilde{\eta}$ is any given number, there exists a unique solution $\tilde{Y}(x)$ of (1.1) where $\tilde{Y}(x)$ is continuous and differentiable for all $\left(x, \tilde{Y}\right)$ in D. The requirement (1.4) is known as Lipschitz condition. See Henrici (1962) for the proof. This assumption establishes the existence of a unique solution of (1.1).

1.3 Stiff ordinary differential equations

Based on Aliyu et al. (2014), the phenomenon of stiffness is not precisely defined in the literature. Some attempts on describing a stiff problem are:

i) A differential equation of the form $y' = f(t, y(t))$ is said to be stiff if its exact solution $y(t)$ includes a term that decays exponentially to zero as t increases, but whose derivatives are much greater in magnitude than the term itself. An example of such a term is $e^{-\lambda t}$, where λ is a large, positive constant, because its k^{th} derivative is $c^k e^{-\lambda t}$. Because of the factor of c^k, this derivative decays to zero much more slowly than $e^{-\lambda t}$ as t increases. Because the error includes a term of this form, evaluated at a time less than t, the error can be quite large if h which is the step size is not chosen sufficiently small to offset this large derivative. Furthermore, the larger λ is, the smaller h must be to maintain accuracy.

ii) A problem is stiff if it contains widely varying time scales where some components of the solution decay much more rapidly than others.
iii) A problem is stiff if the step size is dictated by stability requirements rather than by accuracy requirements.
iv) A problem is stiff if explicit methods do not work or work only extremely slowly.
v) A linear problem is stiff if all of its eigenvalues have negative real part, and the stiffness ratio (the ratio of the magnitudes of the real parts of the largest and smallest eigenvalues) is large.

It is pertinent to note that this thesis follows the definition of stiff problem which is given by Lambert (1991) as follows:

Definition 1.1
The system of (1.1) is said to be stiff if $\mathrm{Re}(\lambda_t) < 0, t = 1,2,\ldots,m$ and $\max_t |\mathrm{Re}(\lambda_t)| \gg \min_t |\mathrm{Re}(\lambda_t)|$ where λ_t are the eigenvalues of the Jacobian matrix, $J = \left(\frac{\partial f}{\partial y}\right)$.

1.4 Linear multistep method

The concept of linear multistep method (LMM) which is developed by Dahlquist (1956) has attracted considerable attention through the exposition by Henrichi (1962, 1963). Hence some definitions of LMM are presented which has been established by Lambert (1991).

Definition 1.2
The general forms of LMM for first and second order ODEs are given as follows:
For first order ODEs:

$$\sum_{j=0}^{k} a_j y_{n+j} = h \sum_{j=0}^{k} b_j y'_{n+j}, \tag{1.5}$$

For second order ODEs:

$$\sum_{j=0}^{k} a_j y_{n+j} = h \sum_{j=0}^{k} b_j y'_{n+j} + h^2 \sum_{j=0}^{k} c_j y''_{n+j}, \tag{1.6}$$

where a_j, b_j and c_j are constants coefficients subject to the conditions $a_k \neq 0$ and not all a_0, b_0, c_0 are zero. k is defined as the order of the method and h is the step size. The method (1.5) is explicit if $b_k = 0$ and it is implicit if $b_k \neq 0$. The associated linear difference operator, L for (1.6) is

$$L\left[y(x);h\right] = \sum_{j=0}^{k} \left[a_j y(x+jh) - h b_j y'(x+jh) - h^2 c_j y''(x+jh) \right], \tag{1.7}$$

where $y(x)$ is an arbitrary function, continuously differentiable on $[a,b]$. The function $y(x)$ may have many higher derivatives. By the Taylor expansion of functions $y(x+jh)$, $y'(x+jh)$ and $y''(x+jh)$ about the point x, and subsequently collecting the derivatives y gives

$$L\left[y(x);h\right]=\sum_{j=0}^{k}\left[C_0 y(x)+C_1 h y'(x)+C_2 h^2 y''(x)+\cdots+C_q h^q y^{(q)}(x)+\cdots\right]. \quad (1.8)$$

The constant C_q is defined as

$$\begin{aligned} C_0 &= \sum_{j=0}^{k} a_j, \\ C_1 &= \sum_{j=0}^{k} (j a_j - b_j), \qquad (1.9) \\ C_q &= \sum_{j=0}^{k}\left(j^q \frac{1}{q!} a_j - j^{q-1}\frac{1}{(q-1)!} b_j - j^{q-2}\frac{1}{(q-2)!} c_j \right), \; q=2,\ 3,\ 4,\ \cdots. \end{aligned}$$

Henrici (1962) stated that the order of the LMM for first and second order ODEs can be determined based on the following definitions.

Definition 1.3
The LMM (1.5) is said to be of order p if $C_0 = C_1 = \ldots = C_p = 0,\ C_{p+1} \neq 0$ where C_{p+1} is error constant.

Definition 1.4
The LMM (1.6) is said to be of order p if $C_0 = C_1 = \ldots = C_p = C_{p+1} = 0,\ C_{p+2} \neq 0$ where C_{p+2} is error constant.

The ability of a method to approximate the exact solutions of differential equations to any required accuracy as the step size tends to zero is called convergence. Bausys (1996) stated that the convergence requires consistency and unconditionally stable which can be determined by the spectral radius. The definition of unconditionally stable is given as follows:

Definition 1.5
The numerical method is unconditionally stable if the spectral radius is less than or equal to unity, $\rho(A) \leq 1$. The spectral radius, ρ of amplification matrix, A is defined by $\rho(A) = \max_i \left|t_i(A).i = 1,2,\ldots,N\right|$ where N is the dimension of amplification matrix, A.

Another alternative definition of convergence has been discussed by Butcher (2008). The author mentioned that the LMM is convergent if and only if it is consistent and zero-stable. The definitions of consistency and zero stability are given as follows:

Definition 1.6
The LMM is consistent if and only if the following conditions are satisfied:

$$\sum_{j=0}^{k} a_j = 0,$$
$$\sum_{j=0}^{k} j a_j = \sum_{j=0}^{k} b_j, \tag{1.10}$$

Definition 1.7
The LMM is said to be zero-stable if no root of the first characteristic polynomial, $p(t)$ has modulus greater than one, and if every root with modulus one is simple.

Shampine and Watts (1969) emphasized that the stability problem would appear to be the most serious limitation of LMM. Therefore, the stability properties of any LMM must be considered to ensure an effectiveness of the solutions. The following definitions demonstrate the absolute stability and A-stable of LMM.

Definition 1.8
The LMM is said to be absolutely stable in a region $\Re$ (real part) of the complex plane if, for all $\hat{h} \in \Re$, all roots of the stability polynomial, $p(t, \hat{h})$ associated with the method, satisfy $|t_s| < 1,\ s = 1,\ 2, \cdots,\ k.$

Definition 1.9
The LMM is A-stable if its region of absolute stability contains the whole of the left-hand half-plane, $\Re(h\lambda) < 0$.

1.5 Objectives

This thesis aims to achieve the following objectives:

i) To derive the constant step block backward differentiation alpha-formulas for solving first and second order stiff ODEs.
ii) To develop the block backward differentiation alpha-formulas using variable step size strategy for solving first and second order stiff ODEs.
iii) To establish the stability and convergence properties of the derived methods.
iv) To compare the performance of the derived methods with the existing methods in terms of accuracy and computational time.
v) To analyze the numerical solutions of damped oscillation problems using the developed methods.

1.6 Scope and Limitation

This thesis concentrates on the derivation of block alpha methods for solving first and second order stiff ODEs. Note that the second order stiff initial value problems (IVPs) of ODEs will be solved directly without reducing it into a system of first order. The proposed methods will be derived using constant step and variable step approach to produce the approximated solutions at two points simultaneously. To evaluate the effectiveness of the derived methods in solving stiff ODEs, the numerical results will be compared with the results obtained in the scientific literature. The comparison parameters consist of the total number of steps, successful steps, failure steps, maximum errors, average errors and computation time. However, the computation time is limited to some numerical results due to the difference environment and equipments. In addition, the under-damped, critically-damped and over-damped oscillation problems of second order IVPs in mass-spring systems are solved to ensure the capability of the derived methods in solving applied problems.

1.7 Framework of the thesis

This chapter begins with a brief background of the thesis followed by some basic concepts of problems considered and relevant definitions which will be referred later in the next chapters.

Chapter 2 gives the summary of earlier numerical methods and reviews some theories and formulation of existing α-methods to support the contribution of the current research.

Chapter 3 presents the derivation of constant step BBDF-α of order three and four for solving first order stiff ODEs. The order of the method is verified. The conditions of consistency and zero stability are satisfied to show the convergence properties of the method. The strategy of choosing the suitable α is presented. In order to show the BBDF-α is A-stable for some values of α, the graph of stability region is plotted. The implementation of the method using Newton iteration is also discussed. The performance of the derived method is compared with the numerical results obtained in the literature.

Chapter 4 focuses on the derivation of variable step BBDF-α of order three and order four for solving first order stiff ODEs. The strategy of varying the step size is discussed. The order, convergence and stability properties of the method are investigated. At the end of this chapter, the numerical results of the derived method are compared with several existing methods and MATLAB's solvers.

In Chapter 5, the constant step BBDF-α is constructed for solving second order stiff ODEs directly. The details derivation and order conditions are described. The convergence properties are verified while the stability region is illustrated. Numerical results and the comparison with several existing methods are provided.

Chapter 6 pays full attention to the derivation of BBDF-α using variable step size strategy for solving second order stiff ODEs directly. The strategy of maintaining or varying the step size ratio is also discussed. The algorithm of the implementation is presented. This chapter ends with the comparison of its performance with the existing methods and MATLAB's solvers.

Numerical solution of damped oscillation problems presented in Chapter 7 relies heavily on the previous chapters. A brief introduction of oscillation problems is discussed. Subsequently, the formulas derived in Chapter 3, 4, 5 and 6 are adopted to deal with under-damped, over-damped and critically-damped oscillation problems in mass-spring systems. Some numerical experiments are presented to demonstrate the capability of the derived methods in solving real-life application. Finally, this thesis is summarized and recommendation for future research is stated in Chapter 8.

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